



# Neither Physics nor Chemistry: A History of Quantum Chemistry

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Alán Aspuru-Guzik

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Peliti's *Statistical Mechanics in a Nutshell*—originally published in Italian (Bollati Boringhieri, 2003)—is a fantastic reference for those who know the subject, teach it, or need a quick technical reminder, especially on the topic of phase transitions, which are consistently featured in modern-day discussions and one that Walecka's book omits. Browsing Peliti's book reminded me of such texts as Kerson Huang's *Statistical Mechanics* (2nd edition, Wiley, 1987); David Chandler's *Introduction to Modern Statistical Mechanics* (Oxford University Press, 1987); and Mehran Kardar's *Statistical Physics of Particles and Statistical Physics of Fields* (both published by Cambridge University Press, 2007).

Of the books under review, *Statistical Mechanics in a Nutshell* provides the more general overview, with topics such as the renormalization group method. It includes a good mix of fundamental thermodynamics, phase behavior, and other key subjects. Even so, I do not see it as a standalone book for introductory students, even if they are energetic and serious; they will need an expert teacher or practitioner to make the ideas become more vivid in the classroom.

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## Introduction to Experimental Biophysics

### Biological Methods for Physical Scientists

Jay Nadeau  
CRC Press, Boca Raton, FL, 2012.  
\$89.95 (641 pp.).  
ISBN 978-1-4398-2953-0

Each year a number of physicists leave various disciplines to become biophysicists. Those converted physicists are challenged to learn various life-science laboratory techniques applicable to molecular biology, microbiology, biochemistry, and cell biology, among other subfields. They also must become familiar with the spectroscopic, microscopic, and other important physical techniques that are now staples of many biological physics labs.

Those challenges highlight the need for effective laboratory manuals, proto-

cols, guides, and other instructional material. Jay Nadeau's *Introduction to Experimental Biophysics: Biological Methods for Physical Scientists* is an ambitious text aimed at educating new graduate students about the important and most common techniques used in a modern biological physics laboratory; it could also serve nicely as a reference manual for advanced graduate students of new or underused protocols. Whereas most existing texts of its kind are aimed at educating biologists or biochemists, Nadeau's is aimed at young biophysicists and more seasoned researchers transferring to the field.

*Introduction to Experimental Biophysics* includes chapters that cover basic concepts behind commonly used biological techniques—for example, transfection, protein purification, and protein crystallography. Other, more physically flavored chapters discuss the concepts behind microscopy, surface chemistry, inorganic nanoparticles, and quantum dots. Each chapter contains protocols and the conceptual reasoning behind them, which is often useful to physicists performing biological experiments for the first time. Specific gems of the book include an overview in chapter 1 of the physical principles common in biological systems; a detailed experimental overview in chapter 5 of x-ray protein crystallization and a useful troubleshooting section to help novices; and a number of extremely useful discussions in chapter 10 on surface modification and functionalization. Surface preparation is particularly important in biophysics: If done incorrectly, it can ruin an otherwise beautiful experiment. The end of each chapter includes extensive references, information about equipment suppliers, helpful websites and software, and additional experimental protocols.

Despite its more than 600 pages, the book is still lacking in some aspects. Perhaps that's not surprising, given its broad scope and ambitious nature. First, most chapters give few details about advanced techniques. For instance, in chapter 6, which covers light microscopy, only one paragraph discusses total internal reflection fluorescence microscopy. Nowhere does the book mention optical or magnetic tweezers, which are used in force spectroscopy and are prevalent in modern biological physics laboratories. Further, various microscopies are discussed in multiple chapters, with electron microscopy (only scanning EM and not transmission EM) addressed in chapter 8 and

atomic force microscopy presented in chapter 10.

The book does not mention techniques that use phospholipids, has insufficient information on chromatographic techniques, and lacks a discussion of the usefulness of centrifugation. New entrants to the field would benefit from learning about the best strategies to extract data—a skill that is not always obvious to beginners—and from knowing the limits of the various techniques, as was done in the troubleshooting section of chapter 5 on protein crystallization and in the example experiments for flow cytometry in chapter 7.

Overall, the many outstanding qualities of *Introduction to Experimental Biophysics* should make it an essential part of the biophysicist's collection. For new students, it is best partnered with the following texts. *At the Bench: A Laboratory Navigator* (Cold Spring Harbor Laboratory Press, 2005), by Kathy Barker, contains useful information about the social forces that shape the establishment of laboratories and how to cope with working in the lab on a daily basis. *And Principles and Techniques of Biochemistry and Molecular Biology* (7th edition, Cambridge University Press, 2010), edited by Keith Wilson and John Walker, provides useful basic information, including a table of units and standard formulas needed to analyze biochemical data.

*Introduction to Experimental Biophysics* assumes readers are already acclimated to the lab and can figure out for themselves how to analyze the data, if only they could get the data using the right biological experimental techniques. This book is likely to become increasingly useful with future editions and iterations, but in its current state, other sources—most likely collaborating biologists—will be required to fill in the gaps.

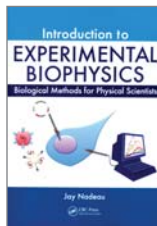
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## Neither Physics nor Chemistry

### A History of Quantum Chemistry

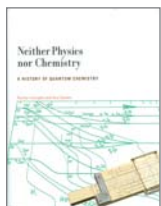
Kostas Gavroglu and Ana Simões  
MIT Press, Cambridge, MA, 2012.  
\$40.00 (351 pp.).  
ISBN 978-0-262-01618-6

The way new areas of science are birthed is similar to the way continental masses are formed: by the contact and





interaction of previously existing structures, which are subsequently modified



so that they never are what they were before. And just as interactions between continental masses lead to tectonic events such as earthquakes and volcanic activity, the gestation

of a new scientific field is usually not smooth.

Quantum chemistry was born in a rocky, volcanic fashion, and the history of its formation has not been covered extensively until now. In *Neither Physics nor Chemistry: A History of Quantum Chemistry*, historians of science Kostas Gavroglu and Ana Simões trace the development of a field that came about through interactions among physics, chemistry, applied mathematics, and what we now call computer science. An illuminating and well-researched book, *Neither Physics nor Chemistry* covers the half-century expansion period of the 1920s to the 1970s, from the era of Walter Heitler and Fritz London through the tensions between the chemists and physicists, between the New World and the Old, and even among the actors in the field with differing political affilia-

tions. The book is full of interesting anecdotes, quotes, and foundational ideas conceived by those players.

*Neither Physics nor Chemistry* parallels *Image and Logic: A Material Culture of Microphysics* (University of Chicago Press, 1997; reviewed by W. K. H. Panofsky in *PHYSICS TODAY*, December 1997, page 65). In *Image and Logic*, author Peter Galison paints a similar multidisciplinary picture of the birth of particle physics. In particular, in a chapter on computer simulation, Galison describes the conceptual "trading zone" between the physicists and computer engineers that, starting in the 1940s, led to the use of the first computers, such as the MANIAC at Los Alamos, to carry out Monte Carlo simulations. The book narrates the visionary work, from around the same time, of chemist Samuel Boys, who used the EDSAC computer in the UK to carry out early quantum chemistry calculations.

The biographies of the heroes of quantum chemistry are less known than those of the founders of quantum mechanics or of the creators of the atomic bomb. Many people know about Wolfgang Pauli or Werner Heisenberg, but fewer know about Hans Hellman or Robert Mulliken. *Neither Physics nor*

*Chemistry* addresses that discrepancy. Moreover, it contains plenty of material about the critical discussions that are still relevant to how chemists work. If one wants to dig to the roots of why organic chemists still think in a "local" valence bonding picture, yet many theoretical chemists are rooted in molecular orbital theory, this book provides the historical context.

Almost a hundred years have passed since the beginnings of quantum chemistry, and both of the parent fields, quantum physics and chemistry, have changed a lot. One thrust of current quantum mechanics is quantum technology: Every day we witness advances in the development of novel devices that could be used for quantum information processing. Meanwhile, theorists are developing new ideas based on quantum information, and experimental physical chemists are using light to probe atoms and molecules at very short times and very high energies. The interaction between 21st-century physics and chemistry might lead either to a renewal of quantum chemistry or to a new field that harvests the current developments from physics and chemistry. Perhaps one might call it quantum information chemistry; that

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may be the subject of a book by future historians, who would do well to be as lucid in their analysis as Gavroglu and Simões have been.

**Alán Aspuru-Guzik**  
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